# ***Proposal for building an ozone module for STICS***

First, we present the way the impact of ozone ($O_3$) was already introduced into new or existing models (Kobayashi, 1997; AFRCWHEAT2-$O_3$ with Ewert and Porter, 2000; Van Oijen et al., 2004 and CERES-$O_3$ model with Lebard, 2005). Second, we discuss the way those approaches feed the conceptual framework of the new ozone module for the STICS model.

## 1. Presentation of existing modelling approaches for $O_3$ effects on crop growth and development

For every approaches, we detail the way (i) the $O_3$ influx into the plant, (ii) the $O_3$ inhibition of photosynthesis and (iii) the $O_3$ acceleration of leaf senescence, are calculated.

### *a. Kobayashi, 1997*

i. $O_3$ inflow

The $O_3$ inflow is not actually calculated. The model consider a **daily damaging O3 concentration** $[O_3](d)$[1] that is calculated as the excess of $O_3$ concentration beyond a background $O_3$ concentration under which there is no damage $P\_[O_{3,b}]$[2]:

$$[O_3](d) = [O_{3,a}](d) - P\_[O_{3,b}] \tag{1}$$

ii. $O_3$ effect on photosynthesis

The daily radiation use efficiency RUE(d) is reduced by a factor accounting for the daily damaging O3 concentration $[O_3](d)$ previously calculated (eq.1). This reducing factor also depends on the sensitivity of the crop to $O_3$, varying with the phenology, P_pi.

$$RUE_{O_3}(d) = \left(1 - P\_pi \cdot [O_3](d)\right) \cdot RUE(d) \tag{2}$$

With P_pi = $P\_p_{veg}$ during vegetative growth, and P_pi = $P\_p_{rep}$ during reproductive growth. $P\_p_{veg}$ is assumed to be lower than $P\_p_{rep}$, considering that the $O_3$ impact on photosynthesis is much greater during reproductive growth.

iii. $O_3$ effect on senescence

The natural senescence rate $P\_\alpha_r$ is increased by a factor accounting for the daily damaging $O_3$ concentration $[O_3](d)$ previously calculated (eq.1). This factor also depends on the sensitivity of the crop to $O_3$ during reproductive growth, $P\_p_{rep}$. The daily LAI is thus calculated after having reached its maximum ($LAI_{max}$):

$$LAI(d) = LAI_{max} - P\_\alpha_r \sum_{LAI_{max}day}^{Harvest\ day} \left(1 + P\_p_{rep} \cdot [O_3](d)\right) \tag{3}$$

### *b. Ewert and Porter with AFRCWHEAT2-O3, 2000*

i. $O_3$ inflow

The **instantaneous $O_3$ uptake rate** $O_{3,up}$ is calculated according to the stomatal conductance for $O_3$ which is the stomatal conductance for $CO_2$ $g_{sc}$ corrected for the differences in the diffusivities of $CO_2$ and $O_3$ in the air with the ratio $P\_f_{DO3}$ (Laisk et al., 1989):

$$O_{3,up} = [O_{3,a}] \cdot g_{sc} \cdot P\_f_{DO3} \tag{4}$$

[1] All parameters and variables are listed in annex 1
[2] All parameters, supposed to remain constant are preceded by "P_"

ii. $O_3$ effect on photosynthesis

The short-term $O_3$ inhibition on photosynthesis is simulated through an $O_3$ dose effect factor $f_{O3,s}$ (d) (see eq.5 below) taking into account that:

- the short-term photosynthesis inhibition $f_{O3,s}$ (d) depends on the damage caused by $O_3$ during the current AND the previous hours $f_{O3,s}$ (h) and $f_{O3,s}$ (h-1) respectively (eq.5);
- there is a dose threshold under which there is no damage (P_γ1/P_γ2 in eq.6);
- the recovery from $O_3$ damage depends on leaf age according to the $f_{LA}$ function (young leaves resist higher $O_3$ concentrations and can recover completely from $O_3$ damage within a period ranging from hours to a few days, Saxe 1991);

$$f_{O3,s}(d) = f_{O3,s}(h) \cdot f_{O3,s}(h-1) \qquad for\ h = 2,3 \ldots 24$$
$$f_{O3,s}(d) = f_{O3,s}(h) \cdot r_{O3,s} \qquad for\ h = 1 \tag{5}$$

With:

$$f_{O3,s}(h) = \begin{Bmatrix} 1 & if\ O_{3,up} \leq P\_\gamma_1/P\_\gamma_2 \\ 1 + P\_\gamma_1 - P\_\gamma_2 \cdot O_{3,up} & if\ P\_\gamma_1/P\_\gamma_2 < O_{3,up} < \frac{1+P\_\gamma_1}{P\_\gamma_2} \\ 0 & if\ O_{3,up} \geq \frac{1+P\_\gamma_1}{P\_\gamma_2} \end{Bmatrix} \tag{6}$$

And:

$$r_{O3,s} = f_{O3,s}(d-1) + [f_{O3,s}(h-1)] \cdot f_{LA} \tag{7}$$

Where $r_{O3,s}$ corresponds to the incomplete recovery from $O_3$ damage of the previous day (considering that repair of ozone damage during the night was not sufficient);

And where $f_{LA}$ is a factor accounting for leaf age, with values between 0 and 1; $f_{LA}$ equals to 1 before emergence, decreases linearly with the age of the leaf (°C.day) and falls to zero when the leaf is dead. Thus before emergence $r_{O3,s}$ =1 and for mature leaves there is quite no repair during the night ($r_{O3,s} \approx f_{O3,s}$ (d-1)) (figure 1).

Finally this short-term photosynthesis inhibition factor $f_{O3,s}$ (d) reduces the Rubisco-limited rate of photosynthesis Ac (simulated at hourly steps as in the biochemical model of photosynthesis developed by Farquhar et al., 1980 and von Caemmerer & Farquhar, 1981):

$$A_{c,O3} = A_c \cdot f_{O3,s}(d) \cdot f_{LS} \tag{8}$$

The $f_{LS}$ term in eq.8 is a senescence factor taking into account the natural decrease of the Rubisco-limited rate of photosynthesis with leaf senescence. As $O_3$ is assumed to accelerate senescence, this $f_{LS}$ term is detailed below.

iii. $O_3$ effect on senescence

$O_3$ is assumed to accelerate the rate of senescence by reducing leaf life-span $t_{l,ma}$ through a long-term $O_3$ impact factor $f_{O3,l}$ calculated as a function of accumulated ozone uptake (till the leaf age $t_l$):

$$f_{O3,l} = 1 - P\_\gamma_3 \int_0^{t_l} O_{3,up} dt$$
$$t_{l,ma} = (t_{l,ep} + t_{l,se}) \cdot f_{O3,l} \tag{10}$$

Where $t_{l,ma}$ is the life-span of a mature leaf, corresponding to the thermal time from sowing to fully expanded leaf stage ($t_{l,ep}$) plus the thermal time during which the leaf is senescing $t_{l,se}$. $O_3$ is thus also assumed to bring forward the onset of senescence ($t_{l,se}$=0.33$t_{l,ma}$ , Porter, 1984).
Finally, the factor $f_{LS}$ accounting for the effect of senescence on the Rubisco-limited rate of photosynthesis Ac, is calculated taking into account the effect of accumulated ozone uptake (eq.11)

$$f_{LS} = \begin{cases} 1 & before\ the \text{ fully expanded leaf } stage \\ 1 - \frac{a_l - t_{l,ep}}{t_{l,ma}/f_{O3,l} - t_{l,ep}} & for\ t_{l,em} < a_l < t_l \\ 0 & for\ a_l \geq t_l \end{cases} \quad (11)$$

Where $a_l$ is the leaf age (°Cday) and $t_l$ is the leaf life-span (°Cday)

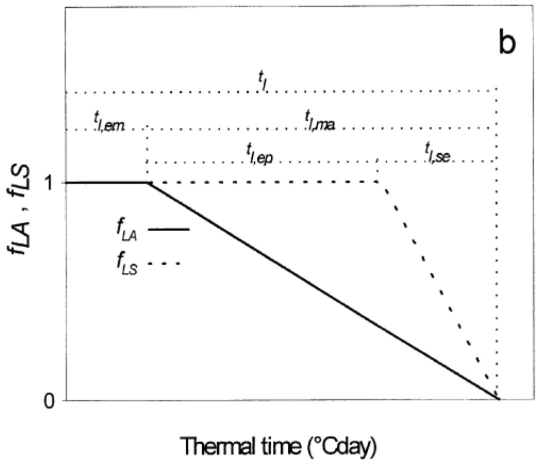


*Figure 1: $f_{LA}$ and $f_{LS}$ factors versus the thermal time (from Ewert & Porter, 2000)*

### *c. Van Oijen et al., 2004*

i. <u>$O_3$ inflow</u>

The **daily damaging $O_3$ uptake** $QO_{3,up}$ is calculated according to the canopy stomatal conductance for CO2 and $O_3$ $g_s$, the photoperiod average of ambient ozone concentration $[O_{3,aph}]$, and taking into account that part of the flux that is detoxified by inert plant material (cell walls) and by biochemical detoxification mechanisms $P\_f_{detox}$:

$$QO_{3,up} = [O_{3,aph}] \cdot g_s \cdot (1 - P\_f_{detox}) \quad (12)$$

ii. <u>$O_3$ effect on photosynthesis</u>

The daily radiation use efficiency RUE(d) is reduced by a factor $F_{O3}(d)$ accounting for the daily photoperiod average of ambient ozone concentration $[O_{3,aph}]$ (and not for the daily damaging O3 uptake previously calculated $QO_{3,up}$ eq.12 !):

$$RUE_{O_3}(d) = RUE(d) \cdot F_{O3}(d) \quad (13)$$

With:

$$F_{O3}(d) = 1 - \frac{44}{30} \frac{[O_{3,aph}] \cdot P\_f_{detox} \cdot P\_c_{detox}}{C_a - C_i} - f_{lv} \cdot P\_f_{repair} \quad (14)$$

Where the ratio 44/30 is the ratio of carbon contents of $CO_2$ (12/44) and $CH_2O$ (12/30), $f_{lv}$ is the fraction of produced assimilates that is allocated to leaf growth and maintenance, $f_{repair}$ is the fraction of assimilates allocated to leaves that is used in repair, $P\_c_{detox}$ is the cost coefficient of detoxification, $C_a$ is ambient $CO_2$ concentration, $C_i$ is the leaf internal $CO_2$ concentration (supposed to be equal to 0.7 $C_a$).

iii. $O_3$ effect on senescence

Nothing is proposed by the authors to deal with the $O_3$ impact on senescence.

### *d. Lebard with CERES-O3, 2005*

i. $O_3$ inflow

The **damaging instantaneous $O_3$ uptake rate within the leaf layer ll $O_{3,up,ll}$** is calculated according to the stomatal conductance for $O_3$, $g_{O3}$, the ambient ozone concentration near leaf surface in the leaf layer ll, $[O_{3,a,ll}]$, and taking into account that a part of the flux is detoxified accordingly to the leaf age:

$$O_{3,up,ll} = ([O_{3,a,ll}] - P\_Kd \cdot Facsen) \cdot g_{O3} \cdot 10^{-12} \quad (15)$$

Where $Kd.g_{O3}.Facsen$ corresponds to the instantaneous detoxified flux in layer ll, and Kd.Facsen is a threshold concentration above which $O_3$ impacts the crop growth. This threshold evolves according to the leaf senescence which is estimated through to ratio between the actual leaf photosynthesis activity and the maximal (before senescence) leaf photosynthesis activity:

$$Facsen = \frac{V_{cmax}}{P\_V_{cmaxopt}} \quad (16)$$

A **damaging cumulative amount of $O_3$** is then calculated (t in second):

$$CO_{3,up,ll} = \int_0^t O_{3,up,ll} \cdot 3600 \cdot dt \quad (17)$$

ii. $O_3$ effect on photosynthesis

The maximum rate of carboxylation $V_{cmax}$ is reduced according to the damaging cumulative amount of $O_3$, $CO_{3,up,ll}$ (eq.17):

$$V_{cmax,O3} = V_{cmax} - P\_Ki \cdot 10^{-3} \cdot CO_{3,up,ll} \quad (18)$$

Where P_Ki is an $O_3$ impact coefficient.

The Rubisco amount is also reduced by the damaging instantaneous $O_3$ uptake rate within the leaf layer ll $O_{3,up,ll}$ calculated as described above (eq.15)

$$\partial RU = -P\_Ki \cdot [RU] \cdot O_{3,up,ll} + \partial RU_{remobilisation} \quad (19)$$

Where $\delta RU$ is the variation of the stock of Rubisco, P_Ki is an impact coefficient (= 302 $s^{-1}$), [RU] is the remaining amount of Rubisco, and $\delta RU_{remobilisation}$ is the reduction of the stock of Rubisco because of remobilization.

This formalism allows simulating the cumulative effect of $O_3$ as well as the dose effect on the photosynthesis response to the cumulative effect (Fig.2).

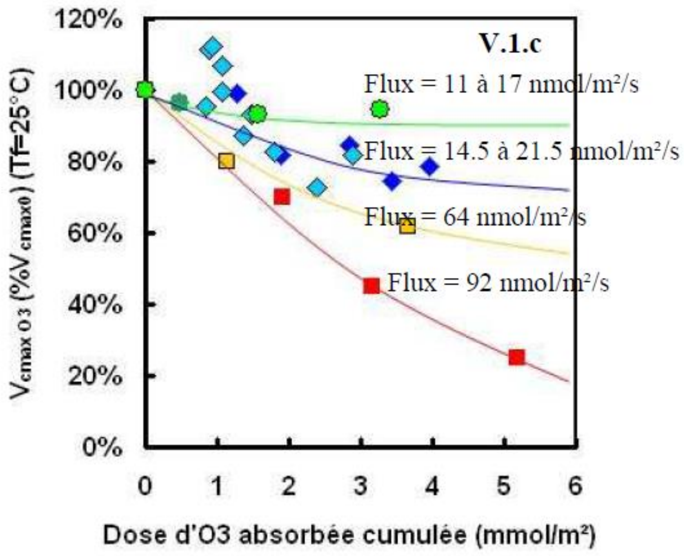


*Figure 2: Maximum carboxylation rate versus cumulative O3 uptake and according to the average O3 inflow (from Lebard, 2005, Fig. V.1.c Chap. V.)*

iii. <u>$O_3$ effect on senescence</u>

Nothing is proposed by the author to deal with the $O_3$ impact on senescence. Furthermore, the author developed a formalism about the $O_3$ impact on leaf nitrogen content.

### e. *Synthesis on about threshold effect, detoxification and repair mechanisms, and time scales which are considered in the previous modelling approaches.*

| Model | O3 Influx | | | O3 impacts | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | Photosynthesis inhibition | | | Senescence acceleration | | |
| | time step and secondary effects | comment | equation | time step and secondary effects | comment | equation | time step and secondary effects | comment | equation |
| Kobayashi (Kobayashi, 1997) | daily<br>threshold effect | The $O_3$ influx is not calculated, but a damaging $[O_3]$ is calculated.<br>the threshold $[O_3]$ air is supposed to be constant | eq. 1 | daily<br>leaf age effect on the repair capacity | 2 sensitivity parameters are fixed, one for the vegetative growth, and one for the reproductive growth | eq. 2<br>eq. 2 | daily | daily senescent rate is increased by daily damaging $O_3$ uptake | eq. 3 |
| AFRCWHEAT2-O3 (Ewert & Porter, 2000) | instantaneous (second) | | eq. 4 | hourly<br>threshold effect<br>leaf age effect on the repair capacity | $O_3$ effect on the Rubisco-limited rate of photosynthesis Ac (FvCB model)<br>low $O_3$ concentration are detoxified without direct effect on the photosynthetic system; but the reduced detoxification capacity with leaf age is not taken into account (Pell et al., 1997)<br>young leaves can recover fully from $O_3$ damage (Pell et al., 1992) | eq. 5<br>eq. 6<br>eq. 7 | daily? | cumulative effect of $O_3$ on senescence | eq. 10 |
| van Oijen (van Oijen et al., 2004) | daily<br>threshold effect | the $O_3$ flux that is instantaneously detoxified is cut away in order to directly calculate a damaging $O_3$ uptake | eq. 12 | daily<br>threshold effect<br>no leaf age effect | $O_3$ effect on the RUE<br>the cost of $O_3$ detoxification is taken into account<br>the cost of leaf repair is taken into account as a constant parameter | eq. 13<br>eq. 14<br>eq. 14 | | | |
| CERES-O3 (Lebard, 2005) | instantaneous (second)<br>threshold effect<br>leaf age effect on instantaneous detoxification (Pell et al., 1997) | The damaging instantaneous $O_3$ uptake rate is calculated for every leaf layers | eq. 15 | hourly | damaging $O_3$ cumulative amount effect on the maximum rate of carboxylation Vcmax (FvCB model) | eq. 18 | | | |

## 2. Conceptual framework of the future STICS $O_3$ module

In order to build an O3 module pluggable to STICS, it's necessary to choose formalisms using input variables that can be provided by STICS (or at less calculated from STICS state variables). As STICS assesses daily canopy resistances for $CO_2$ exchanges through a resistive approach (Fig. 3), and simulates a daily net photosynthesis according to an integrative approach without downscaling to the biochemical processes such as in the FvCB model, we propose the following formalisms in line with van Oijen et al. (2004) and Lebart (2005).

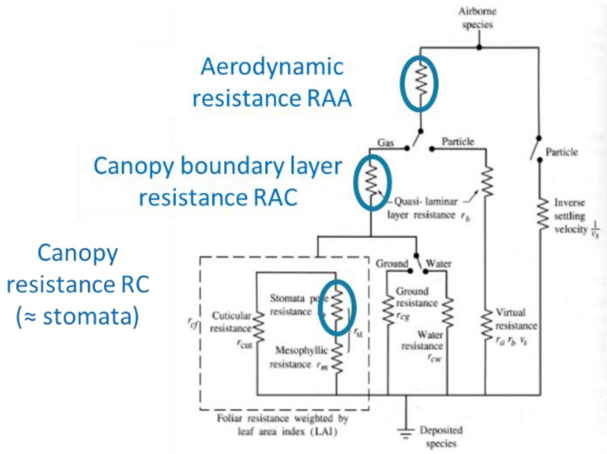


*Figure 3: Canopy resistances as calculated by STICS (from Brisson et al., 2009)*

### *a. O3 inflow*

In line with van Oijen et al. (2004), the **daily damaging $O_3$ uptake $QO_{3,up}$** (nmol.m$^{-2}$ ground.day$^{-1}$) is calculated according to the canopy resistance for $O_3$ (the inverse of canopy conductance for $O_3$), the photoperiod average of ambient ozone concentration [$O_{3,aph}$] (nmol.m$^{-2}$ ground.s$^{-1}$), and taking into account that part of the flux that is instantaneously detoxified $P\_f_{detox}$ (eq. 20). The canopy resistance for $O_3$ is the canopy resistance for $CO_2$ RT (sm$^{-1}$) corrected for the differences in the diffusivities of $CO_2$ and $O_3$ in the air with the ratio $P\_kdif_{O3}$ (eq. 20). Two options were implemented, considering only the stomatal resistance rc (1$^{st}$ option) which is the greater contribution, or alternatively all resistances (2$^{nd}$ option) i.e. aerodynamic resistance raa, canopy boundary layer resistance rac and stomatal resistance rc (eq. 21):

$$QO_{3,up}(d) = 1/RT(d) \cdot [O_{3,aph}] \cdot P\_kdif_{O3} \cdot (1 - P\_f_{detox}) \cdot photoperiod \cdot 3600 \qquad (20)$$

Where

$$RT(d) = \begin{cases} rc(d) & if\ option\ 1 \\ rc(d) + rac(d) + raa(d) & if\ option\ 2 \end{cases} \qquad (21)$$

The **damaging cumulative amount of $O_3$ $CO_{3,up}$** (mmol $O_3$ m$^{-2}$ground) is thus equal to:

$$CO_{3,up}(d) = \int_{em}^{d} QO_{3,up}(i) \cdot 10^{-6} \qquad (22)$$

### *b. O3 impact on photosynthesis*

In line with Lebard (2005), we consider the cumulative effect of $O_3$ on photosynthesis, as well as the dose effect on the photosynthesis response to the cumulative effect. We apply Lebard approach (eq.18, fig.2) to the maximum value of the radiation use efficiency EBMAX (eq. 23, Fig. 4):

$$\frac{EBMAX_{O3}(d)}{EBMAX(d)} = 1 - \left(1 - exp\left(-f_{FO3} \cdot CO_{3,up}(d)\right)\right) \tag{23}$$

With :
$$f_{FO3} = P\_kdose_{O3} \cdot FO_{3,up}(d) \tag{24}$$

Where:
$$FO_{3,up} = QO_{3,up}/(photoperiod \cdot 3600) \tag{25}$$

EBMAXO3 is the maximum radiation use efficiency under $O_3$ effect (g biomass.$MJ^{-1}$) while EBMAX is the maximum radiation use efficiency without $O_3$ effect. $CO_{3,up}$ as calculated in eq.22, represents the cumulative amount of $O_3$ uptake, whereas $f_{FO3}$ is the $O_3$ dose effect factor on photosynthesis response to the cumulative effect of $O_3$. $f_{FO3}$ is calculated from $FO_{3,up}$ (eq.24) i.e. the instantaneous average of $O_3$ inflow calculated from the daily damaging $O_3$ uptake $QO_{3,up}$ (eq.25). $P\_kdose_{O3}$ is a coefficient supposed to be constant.

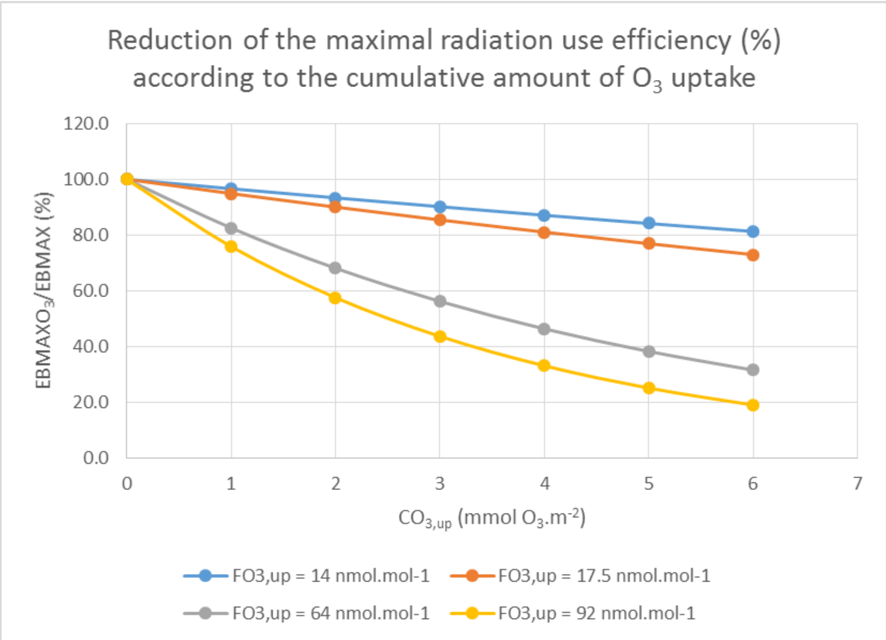


*Figure 4: Relation between the reduction of the maximum radiation use efficiency and the cumulative amount of O3 uptake, according to the inflow intensity*

## 3. <u>Parameterization, evaluation and perspectives of the STICS O3 module</u>

Parameters of the O3 module should now be estimated:

- The ratio of diffusion rates **P_kdifO3** is fixed at 0.93 when considering only the stomatal resistance (1st option), according to Ewert and Porter (2000). When considering all resistances (2nd option) i.e. aerodynamic resistance raa, canopy boundary layer resistance rac and stomatal resistance rc, we should estimate a diffusion ratio for each of them: the diffusion ratio for aerodynamic resistance could be fixed at 1 (A. Olioso, com. Pers.), and the diffusion ratio for boundary layer resistance should be found in the literature.
- The instantaneous detoxified fraction of $O_3$ flux $\mathbf{P\_f_{detox}}$ is fixed at 0.9 according to van Oijen et al. (2004).
- The coefficient for the $O_3$ dose effect factor calculation $\mathbf{P\_kdose_{O3}}$ is estimated from the $VcmaxO_3/Vcmax$ curve by Lebard (2005) originally established with data from Lebard (2005), Farage et al. (1991) and Cardoso Vilhena et al. (2004) (see Lebard, 2005, Figure V.1). The optimized value of $P\_kdose_{O3}$ is thus fixed at $3.10^{-3}$.

The O3 module should be evaluated, and parameters estimated more accurately, according to data found in the literature (such as Farage et al., 1991, Ewert et al., 1999; Cardoso Vilhena et al., 2004 and Lebard, 2005) and from the ozone experiments conducted by Danish colleagues in Roskilde University and DTU within the Climate CAFÉ project (Hansen et al., 2019).

Finally, the effect of leaf age on the detoxification efficiency could be introduced into the module, by transforming the $P\_f_{detox}$ parameter into a variable evolving with leaf age. Last, the effect of $O_3$ on senescence has to be formalized.

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# Annex 1: Table of Parameters, Input and Output variables in models from Kobayashi (1997), Ewert and Porter (2000), van Oijen et al. (2004) and Lebard (2005).

| Name | Input variable / Output variable / Parameter | Definition | Unit | Value (for parameters only) | Equation | Model / Reference | Time step calculation |
|---|---|---|---|---|---|---|---|
| $[O_3](d)$ | Output variable | Daily mean $O_3$ concentration in excess of background $O_3$ (day d) | ppb or $nmol.mol^{-1}$ | | 1 | Kobayashi, 1997 | daily average |
| $[O_{3,a}]$ (d) | Input variable | Daily mean O3 concentration in the air (day d) | ppb or $nmol.mol^{-1}$ | | 1 | Kobayashi, 1997 | daily average |
| $P\_[O_{3,b}]$ | Parameter | Background O3 concentration (under which there is no damage) | ppb or $nmol.mol^{-1}$ | not estimated by author | 1 | Kobayashi, 1997 | |
| RUE(d) | Input variable | Daily radiation use efficiency with no $O_3$ impact | g $biomass.MJ^{-1}$ | | 2 | Kobayashi, 1997 | daily |
| $RUE_{O3}(d)$ | Output variable | Daily radiation use efficiency reduced by $O_3$ impact | g $biomass.MJ^{-1}$ | | 2 | Kobayashi, 1997 | daily |
| $P\_p_{veg}$ | Parameter | sensitivity of photosynthesis to excess $O_3$ during vegetative growth | - | not estimated by author | 2 | Kobayashi, 1997 | |
| $P\_p_{rep}$ | Parameter | sensitivity of photosynthesis and senescence to excess $O_3$ during reproductive growth | - | not estimated by author | 2 | Kobayashi, 1997 | |
| LAI(d) | Output variable | Daily LAI | m2 leaves . $m^{-2}$ soil | | 3 | Kobayashi, 1997 | daily |
| LAImax | Input variable | maximum LAI | m2 leaves . $m^{-2}$ soil | | 3 | Kobayashi, 1997 | crop season maximum |
| $P\_\alpha_r$ | Parameter | constant rate of LAI decrease from the end of vegetative growth (<=> senescence) | - | not estimated by author | 3 | Kobayashi, 1997 | |
| $O_{3,up}$ | Output variable | Instantaneous $O_3$ uptake rate (flux) | $nmol.m^{-2}.s^{-1}$ | | 4 | Ewert&Porter, 2000 | instantaneous (second) |
| $[O_{3,a}]$ | Input variable | Instantaneous $O_3$ concentration at the leaf surface | ppb or $nmol.mol^{-1}$ | | 4 | Ewert&Porter, 2000 | hourly average |
| $g_{sc}$ | Input variable | Stomatal conductance for $CO_2$ | $mol.m^{-2}.s^{-1}$ | | 4 | Ewert&Porter, 2000 | hourly |
| $P\_f_{DO3}$ | Parameter | ratio of diffusion rates for O3 and CO2 | - | 0.93 | 4 | Ewert&Porter, 2000 | |
| $f_{O3,s}(d)$ | Output variable | short-term $O_3$ dose effect factor [0,1] inhibiting photosynthesis and accounting for the damage caused during the current and previous hours | - | | 5 | Ewert&Porter, 2000 | hourly |
| $f_{O3,s}(h)$ | Output variable | short-term $O_3$ dose effect factor [0,1] accounting for the damage caused during the current hour | - | | 5 | Ewert&Porter, 2000 | hourly |
| $P\_\gamma1$ | Parameter | $O_3$ short-term damage coefficient | - | 0.06 | 6 | Ewert&Porter, 2000 | |
| $P\_\gamma2$ | Parameter | $O_3$ short-term damage coefficient | $(nmol.m^{-2}.s^{-1})^{-1}$ | 0.0045 | 6 | Ewert&Porter, 2000 | |
| $P\_\gamma3$ | Parameter | $O_3$ long-term damage coefficient | $(nmol.m^{-2}.s^{-1})^{-1}$ | 0.5 | 10 | Ewert&Porter, 2000 | |
| $A_{C,O3}$ | Output variable | Rubisco-limited rate of carboxylation (during photosynthesis) reduced by O3 effect | $\mu mol.m^{-2}.s^{-1}$ | | 8 | Ewert&Porter, 2000 | instantaneous (second) |
| $A_C$ | Output variable | Rubisco-limited rate of carboxylation (during photosynthesis) | $\mu mol.m^{-2}.s^{-1}$ | | 8 | Ewert&Porter, 2000 | instantaneous (second) |
| $f_{LA}$ | Output variable | factor accounting for leaf age [0,1] | - | | 7 | Ewert&Porter, 2000 | daily |
| $f_{LS}$ | Output variable | factor accounting for leaf senescence [0,1] | - | | 8, 11 | Ewert&Porter, 2000 | daily |
| $t_{l,ma}$ | Output variable | life-span of a mature leaf | °C.day | | 10, 11 | Ewert&Porter, 2000 | daily |
| $t_{l,ep}$ | Input variable | thermal time from sowing to fully expanded leaf stage | °C.day | | 10, 11 | Ewert&Porter, 2000 | daily |
| $t_{l,em}$ | Input variable | thermal time from sowing to emergence | °C.day | | 10, 11 | Ewert&Porter, 2000 | daily |
| $t_{l,se}$ | Input variable | thermal time during which the leaf is senescing | °C.day | | 10 | Ewert&Porter, 2000 | daily |
| $f_{O3,l}$ | Output variable | long-term $O_3$ impact factor [0,1] accelerating senescence | - | | 10 | Ewert&Porter, 2000 | daily |
| $t_l$ | Output variable | life-span of the leaf | °C.day | | 10 | Ewert&Porter, 2000 | daily |
| $a_l$ | Output variable | leaf age | °C.day | | 11 | Ewert&Porter, 2000 | daily |
| $P\_f_{detox}$ | Parameter | detoxified fraction of $O_3$ flux | - | 0.9 | 12 | van Oijen et al., 2004 | daily |
| $QO_{3,up}$ | Output variable | Daily damaging $O_3$ uptake rate (flux) | g $O_3.m^{-2}$ $ground.day^{-1}$ | | 12 | van Oijen et al., 2004 | daily |
| $g_s$ | Input variable | Stomatal conductance for $CO_2$ and O3 (supposed to be equal) | $mol.m^{-2}.s^{-1}$ | | 12 | van Oijen et al., 2004 | instantaneous (second) |
| $[O_{3,aph}]$ | Input variable | photoperiod average of ambient ozone concentration | ml $O_3.m^{-3}$ | | 12 | van Oijen et al., 2004 | daily average |
| RUE(d) | Input variable | Daily radiation use efficiency with no $O_3$ impact | g $biomass.MJ^{-1}$ | | 13 | van Oijen et al., 2004 | daily |
| $RUE_{O3}(d)$ | Output variable | Daily radiation use efficiency reduced by $O_3$ impact | g $biomass.MJ^{-1}$ | | 13 | van Oijen et al., 2004 | daily |
| $F_{O3}(d)$ | Output variable | $O_3$ effect factor [0,1] inhibiting photosynthesis | - | | 13 | van Oijen et al., 2004 | daily |
| $P\_c_{detox}$ | Parameter | cost coefficient of detoxification | g $CH_2O$ $g^{-1}$ detoxifiec | 0.375 | 14 | van Oijen et al., 2004 | |
| $f_{LV}$ | Input variable | fraction of assimilates allocated to leaf growth and maintenance | $g.g^{-1}$ | | 14 | van Oijen et al., 2004 | daily |
| $P\_f_{repair}$ | Parameter | fraction of assimilates allocated to leaves that is used in repair | $g.g^{-1}$ | 0.05 | 14 | van Oijen et al., 2004 | |
| Ca | Input variable | ambient $CO_2$ concentration | ml $CO_2$ $m^{-3}$ | | 14 | van Oijen et al., 2004 | daily |
| Ci | Input variable | leaf internal $CO_2$ concentration | ml $CO_2$ $m^{-3}$ | | 14 | van Oijen et al., 2004 | daily |
| $O_{3,up,ll}$ | Output variable | Damaging instantaneous $O_3$ uptake rate within the leaf layer ll (flux) | $nmol.m^{-2}.s^{-1}$ | | 15 | Lebard, 2005 | instantaneous (second) |
| $[O_{3,a,ll}]$ | Input variable | Instantaneous $O_3$ concentration at the leaf surface in leaf layer ll | ppb or $nmol.mol^{-1}$ | | 15 | Lebard, 2005 | hourly average |
| P_Kd | Parameter | Coefficient of instantaneous detoxification and repair | ppb or $nmol.mol^{-1}$ | 49.4 | 15 | Lebard, 2005 | |
| Facsen | Output variable | Factor of senescence effect on the threshold of damaging instantaneous O3 uptake | - | | 15 | Lebard, 2005 | instantaneous (second) |
| $V_{Cmax,O3}$ | Output variable | Maximum rate of carboxylation reduced by absorbed $O_3$ | $\mu mol.m^{-2}$ $leaf.s^{-1}$ | | 18 | Lebard, 2005 | instantaneous (second) |
| $V_{Cmax}$ | Output variable | Maximum rate of carboxylation | $\mu mol.m^{-2}$ $leaf.s^{-1}$ | | 16 | Lebard, 2005 | instantaneous (second) |
| $P\_V_{cmaxopt}$ | Parameter | Maximum rate of carboxylation for an optimum nitrogen content in leaves | $\mu mol.m^{-2}$ $leaf.s^{-1}$ | 95 | 16 | Lebard, 2005 | instantaneous (second) |
| CO3,up,ll | Output variable | Damaging cumulative amount of uptaken $O_3$ | $mmol.m^{-2}$ leaf | | 17 | Lebard, 2005 | over the crop season |
| P_Ki | Parameter | Coefficient of $O_3$ impact | $s^{-1}$ | 302 | 18 | Lebard, 2005 | |

# Annex 2: Table of Parameters, Input and Output variables of the STICS O3 module

| Name | Input variable / Output variable / Parameter | Definition | Unit | Value (for parameters only) | Equation | Comment |
|---|---|---|---|---|---|---|
| $QO_{3,up}$ | Output variable | Daily damaging $O_3$ uptake | nmol O3.$m^{-2}$ ground.$day^{-1}$ | | 20 | |
| RT | Input variable | Canopy resistance for $CO_2$ | $(mol.m^{-2}.s^{-1})^{-1}$ | | 20, 21 | |
| $[O_{3,aph}]$ | Input variable | photoperiod average of ambient ozone concentration | nmol.$mol^{-1}$ or ppb | | 20 | |
| $P\_kdif_{O3}$ | Parameter | ratio of diffusion rates for $O_3$ and $CO_2$ | - | 0.93 | 20 | From Ewert & Porter (2000) |
| $P\_f_{detox}$ | Parameter | detoxified fraction of $O_3$ flux | - | 0.9 | 20 | From van Oijenet al. (2004) |
| photoperiod | Input variable | Daily interval period during which the plants are exposed to light | hour | | 20, 25 | |
| RT | Input variable | Canopy resistance for $CO_2$ | $(mol.m^{-2}.s^{-1})^{-1}$ | | 21 | |
| rc | Input variable | Stomatal resistance for $CO_2$ | $(mol.m^{-2}.s^{-1})^{-1}$ | | 21 | |
| raa | Input variable | Aerodynamic resistance for $CO_2$ | $(mol.m^{-2}.s^{-1})^{-1}$ | | 21 | |
| rac | Input variable | Boundary layer resistance for $CO_2$ | $(mol.m^{-2}.s^{-1})^{-1}$ | | 21 | |
| $CO_{3,up}$ | Output variable | Damaging cumulative amount of $O_3$ uptake | mmol O3.$m^{-2}$ ground | | 22 | |
| $EBMAX_{O3}$ | Output variable | Maximum radiation use efficiency under $O_3$ effect | g biomass.$MJ^{-1}$ | | 23 | |
| EBMAX | Input variable | Maximum radiation use efficiency without $O_3$ | g biomass.$MJ^{-1}$ | | 23 | |
| fFO3 | Output variable | O3 dose effect factor on photosynthesis response to the cumulative effect of $O_3$ | (mmol O3.$m^{-2}$ ground$)^{-1}$ | | 23, 24 | |
| P_kdoseO3 | Parameter | coefficient for the O3 dose effect factor calculation | $10^6$.(nmol O3$)^{-1}$.$m^4$ ground.day | 0.003 | 24 | estimated from Lebard (2005) with data from Lebard (2005) and Farage et al. (1991) and Cardoso Vilhena et al. (2004) |
| $FO_{3,up}$ | Output variable | Instantaneous damaging $O_3$ uptake rate (flux) | nmol O3.$m^{-2}$ ground.$s^{-1}$ | | 25 | |